From Atomic Structure to Photovoltaic Properties in CdTe Solar Cells

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Scanning transmission electron microscopy (STEM) and electron energy loss spectroscopy (EELS) have been used to determine the atomic structure and Composition of intra-grain dislocations and grain boundaries (GBs) in CdTe. Atomic structure models have been constructed based on the structure observed in STEM. Density functional theory (DFT) calculations show that intra-grain dislocation pairs do *not* create deep states inside the band gap, but instead, induce a significant energy band bending, which could actually reduce electron-hole recombination.

In CdCl2 heat treated CdTe we have used EELS to investigate possible Cl segregation. No Cl enrichment has been detected at simple partial dislocation pairs. However Cl clearly segregates at complex partials, which have a CdTe3 or Cd3Te configuration at the cores. Moreover, a row of Cd3Te core structures have been seen at a Σ9 coincident site lattice GB. Significant Cl enrichment and Te depletion have been found at both the Σ9 GB and random GBs. The electrical activity of the dislocation structures is being studied via DFT calculations.

A cathodoluminescence and electron beam induced current system has been integrated into an aberration-corrected STEM to correlate the electrical and optical properties of individual defects with atomic structure and composition. Initial results will be presented.

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